



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2016 – 02:33 PM EDT

PDB ID : 5FOF
Title : Crystal structure of the P.knowlesi cytosolic leucyl-tRNA synthetase editing domain
Authors : Palencia, A.; Sonoiki, E.; Guo, D.; Ah Yong, V.; Dong, C.; Li, X.; Hernandez, V.S.; Gut, J.; Legac, J.; Cooper, R.; Alley, M.R.K.; Freund, Y.R.; DeRisi, J.; Cusack, S.; Rosenthal, P.J.
Deposited on : 2015-11-19
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

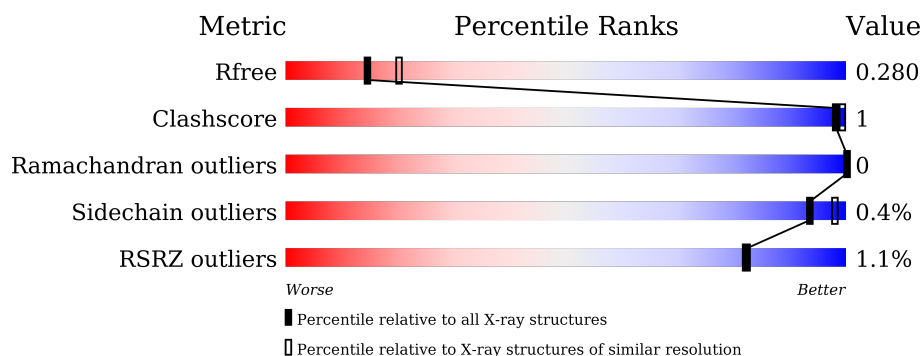
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	330	<div> <div>88%</div> <div>8%</div> </div>
1	B	330	<div> <div>85%</div> <div>12%</div> </div>
1	C	330	<div> <div>87%</div> <div>9%</div> </div>
1	D	330	<div> <div>89%</div> <div>8%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10015 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called LEUCYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2490	1606	394	473	17			
1	B	290	Total	C	N	O	S	0	1	0
			2395	1544	379	455	17			
1	C	299	Total	C	N	O	S	0	0	0
			2464	1588	389	470	17			
1	D	302	Total	C	N	O	S	0	0	0
			2490	1606	394	473	17			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	238	MET	-	EXPRESSION TAG	UNP B3L7I1
A	239	LEU	-	EXPRESSION TAG	UNP B3L7I1
A	240	HIS	-	EXPRESSION TAG	UNP B3L7I1
A	241	HIS	-	EXPRESSION TAG	UNP B3L7I1
A	242	HIS	-	EXPRESSION TAG	UNP B3L7I1
A	243	HIS	-	EXPRESSION TAG	UNP B3L7I1
A	244	HIS	-	EXPRESSION TAG	UNP B3L7I1
A	245	HIS	-	EXPRESSION TAG	UNP B3L7I1
A	246	PRO	-	EXPRESSION TAG	UNP B3L7I1
A	247	MET	-	EXPRESSION TAG	UNP B3L7I1
A	248	SER	-	EXPRESSION TAG	UNP B3L7I1
A	249	ASP	-	EXPRESSION TAG	UNP B3L7I1
A	250	TYR	-	EXPRESSION TAG	UNP B3L7I1
A	251	ASP	-	EXPRESSION TAG	UNP B3L7I1
A	252	ILE	-	EXPRESSION TAG	UNP B3L7I1
A	253	PRO	-	EXPRESSION TAG	UNP B3L7I1
A	254	THR	-	EXPRESSION TAG	UNP B3L7I1
A	255	THR	-	EXPRESSION TAG	UNP B3L7I1
A	256	GLU	-	EXPRESSION TAG	UNP B3L7I1
A	257	ASN	-	EXPRESSION TAG	UNP B3L7I1
A	258	LEU	-	EXPRESSION TAG	UNP B3L7I1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	259	TYR	-	EXPRESSION TAG	UNP B3L7I1
A	260	PHE	-	EXPRESSION TAG	UNP B3L7I1
A	261	GLN	-	EXPRESSION TAG	UNP B3L7I1
A	262	GLY	-	EXPRESSION TAG	UNP B3L7I1
A	263	ALA	-	EXPRESSION TAG	UNP B3L7I1
A	264	MET	-	EXPRESSION TAG	UNP B3L7I1
A	265	GLY	-	EXPRESSION TAG	UNP B3L7I1
B	238	MET	-	EXPRESSION TAG	UNP B3L7I1
B	239	LEU	-	EXPRESSION TAG	UNP B3L7I1
B	240	HIS	-	EXPRESSION TAG	UNP B3L7I1
B	241	HIS	-	EXPRESSION TAG	UNP B3L7I1
B	242	HIS	-	EXPRESSION TAG	UNP B3L7I1
B	243	HIS	-	EXPRESSION TAG	UNP B3L7I1
B	244	HIS	-	EXPRESSION TAG	UNP B3L7I1
B	245	HIS	-	EXPRESSION TAG	UNP B3L7I1
B	246	PRO	-	EXPRESSION TAG	UNP B3L7I1
B	247	MET	-	EXPRESSION TAG	UNP B3L7I1
B	248	SER	-	EXPRESSION TAG	UNP B3L7I1
B	249	ASP	-	EXPRESSION TAG	UNP B3L7I1
B	250	TYR	-	EXPRESSION TAG	UNP B3L7I1
B	251	ASP	-	EXPRESSION TAG	UNP B3L7I1
B	252	ILE	-	EXPRESSION TAG	UNP B3L7I1
B	253	PRO	-	EXPRESSION TAG	UNP B3L7I1
B	254	THR	-	EXPRESSION TAG	UNP B3L7I1
B	255	THR	-	EXPRESSION TAG	UNP B3L7I1
B	256	GLU	-	EXPRESSION TAG	UNP B3L7I1
B	257	ASN	-	EXPRESSION TAG	UNP B3L7I1
B	258	LEU	-	EXPRESSION TAG	UNP B3L7I1
B	259	TYR	-	EXPRESSION TAG	UNP B3L7I1
B	260	PHE	-	EXPRESSION TAG	UNP B3L7I1
B	261	GLN	-	EXPRESSION TAG	UNP B3L7I1
B	262	GLY	-	EXPRESSION TAG	UNP B3L7I1
B	263	ALA	-	EXPRESSION TAG	UNP B3L7I1
B	264	MET	-	EXPRESSION TAG	UNP B3L7I1
B	265	GLY	-	EXPRESSION TAG	UNP B3L7I1
C	238	MET	-	EXPRESSION TAG	UNP B3L7I1
C	239	LEU	-	EXPRESSION TAG	UNP B3L7I1
C	240	HIS	-	EXPRESSION TAG	UNP B3L7I1
C	241	HIS	-	EXPRESSION TAG	UNP B3L7I1
C	242	HIS	-	EXPRESSION TAG	UNP B3L7I1
C	243	HIS	-	EXPRESSION TAG	UNP B3L7I1
C	244	HIS	-	EXPRESSION TAG	UNP B3L7I1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	245	HIS	-	EXPRESSION TAG	UNP B3L7I1
C	246	PRO	-	EXPRESSION TAG	UNP B3L7I1
C	247	MET	-	EXPRESSION TAG	UNP B3L7I1
C	248	SER	-	EXPRESSION TAG	UNP B3L7I1
C	249	ASP	-	EXPRESSION TAG	UNP B3L7I1
C	250	TYR	-	EXPRESSION TAG	UNP B3L7I1
C	251	ASP	-	EXPRESSION TAG	UNP B3L7I1
C	252	ILE	-	EXPRESSION TAG	UNP B3L7I1
C	253	PRO	-	EXPRESSION TAG	UNP B3L7I1
C	254	THR	-	EXPRESSION TAG	UNP B3L7I1
C	255	THR	-	EXPRESSION TAG	UNP B3L7I1
C	256	GLU	-	EXPRESSION TAG	UNP B3L7I1
C	257	ASN	-	EXPRESSION TAG	UNP B3L7I1
C	258	LEU	-	EXPRESSION TAG	UNP B3L7I1
C	259	TYR	-	EXPRESSION TAG	UNP B3L7I1
C	260	PHE	-	EXPRESSION TAG	UNP B3L7I1
C	261	GLN	-	EXPRESSION TAG	UNP B3L7I1
C	262	GLY	-	EXPRESSION TAG	UNP B3L7I1
C	263	ALA	-	EXPRESSION TAG	UNP B3L7I1
C	264	MET	-	EXPRESSION TAG	UNP B3L7I1
C	265	GLY	-	EXPRESSION TAG	UNP B3L7I1
D	238	MET	-	EXPRESSION TAG	UNP B3L7I1
D	239	LEU	-	EXPRESSION TAG	UNP B3L7I1
D	240	HIS	-	EXPRESSION TAG	UNP B3L7I1
D	241	HIS	-	EXPRESSION TAG	UNP B3L7I1
D	242	HIS	-	EXPRESSION TAG	UNP B3L7I1
D	243	HIS	-	EXPRESSION TAG	UNP B3L7I1
D	244	HIS	-	EXPRESSION TAG	UNP B3L7I1
D	245	HIS	-	EXPRESSION TAG	UNP B3L7I1
D	246	PRO	-	EXPRESSION TAG	UNP B3L7I1
D	247	MET	-	EXPRESSION TAG	UNP B3L7I1
D	248	SER	-	EXPRESSION TAG	UNP B3L7I1
D	249	ASP	-	EXPRESSION TAG	UNP B3L7I1
D	250	TYR	-	EXPRESSION TAG	UNP B3L7I1
D	251	ASP	-	EXPRESSION TAG	UNP B3L7I1
D	252	ILE	-	EXPRESSION TAG	UNP B3L7I1
D	253	PRO	-	EXPRESSION TAG	UNP B3L7I1
D	254	THR	-	EXPRESSION TAG	UNP B3L7I1
D	255	THR	-	EXPRESSION TAG	UNP B3L7I1
D	256	GLU	-	EXPRESSION TAG	UNP B3L7I1
D	257	ASN	-	EXPRESSION TAG	UNP B3L7I1
D	258	LEU	-	EXPRESSION TAG	UNP B3L7I1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	259	TYR	-	EXPRESSION TAG	UNP B3L7I1
D	260	PHE	-	EXPRESSION TAG	UNP B3L7I1
D	261	GLN	-	EXPRESSION TAG	UNP B3L7I1
D	262	GLY	-	EXPRESSION TAG	UNP B3L7I1
D	263	ALA	-	EXPRESSION TAG	UNP B3L7I1
D	264	MET	-	EXPRESSION TAG	UNP B3L7I1
D	265	GLY	-	EXPRESSION TAG	UNP B3L7I1

- Molecule 2 is water.

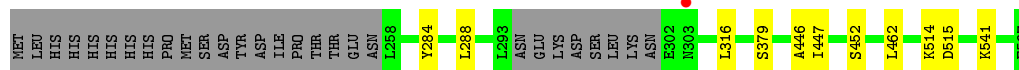
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	47	Total O 47 47	0	0
2	B	53	Total O 53 53	0	0
2	C	35	Total O 35 35	0	0
2	D	41	Total O 41 41	0	0

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

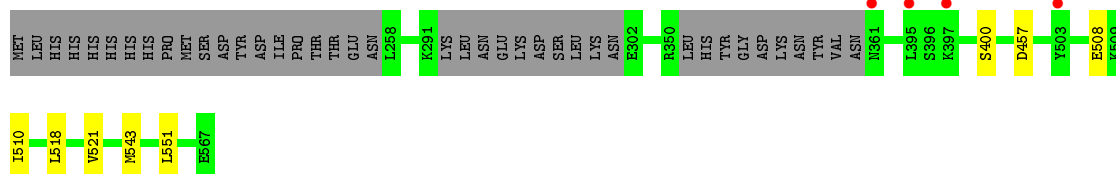
• Molecule 1: LEUCYL-TRNA SYNTHETASE

Chain A: 




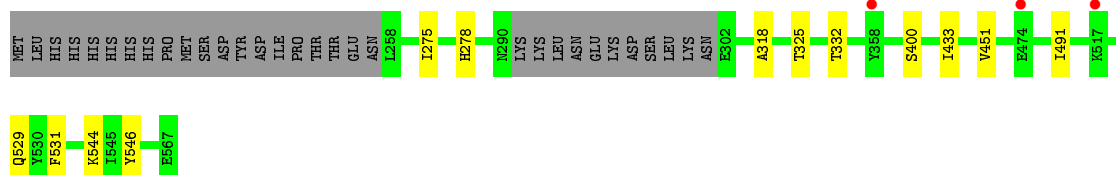
• Molecule 1: LEUCYL-TRNA SYNTHETASE

Chain B: 



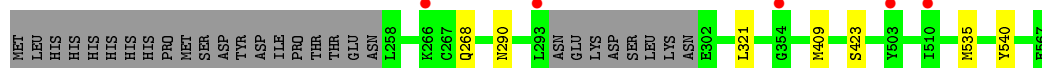
• Molecule 1: LEUCYL-TRNA SYNTHETASE

Chain C: 



• Molecule 1: LEUCYL-TRNA SYNTHETASE

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.03Å 96.82Å 168.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.46 – 2.40 48.31 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (84.46-2.40) 99.7 (48.31-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.218 , 0.280 0.220 , 0.280	Depositor DCC
R_{free} test set	3066 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.656	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 27.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10015	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.48	0/2542	0.65	0/3419
1	B	0.49	0/2446	0.67	0/3287
1	C	0.49	0/2516	0.64	0/3386
1	D	0.49	0/2542	0.65	0/3419
All	All	0.49	0/10046	0.65	0/13511

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2490	0	2470	7	0
1	B	2395	0	2381	5	0
1	C	2464	0	2433	6	0
1	D	2490	0	2470	3	0
2	A	47	0	0	0	0
2	B	53	0	0	0	0
2	C	35	0	0	0	0
2	D	41	0	0	0	0
All	All	10015	0	9754	20	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (20) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:ILE:HD12	1:C:318:ALA:HB2	1.77	0.66
1:A:452:SER:HB3	1:A:462:LEU:HD12	1.81	0.61
1:B:510:ILE:HD11	1:B:521:VAL:HG21	1.85	0.59
1:A:452:SER:CB	1:A:462:LEU:HD12	2.42	0.50
1:B:508:GLU:HG3	1:B:521:VAL:HG22	1.93	0.50
1:C:325:THR:HG22	1:C:491:ILE:CD1	2.42	0.49
1:A:284:TYR:CZ	1:A:288:LEU:HD21	2.48	0.48
1:D:290:ASN:HB2	1:D:409:MET:HE1	1.96	0.47
1:D:268:GLN:HG2	1:D:321:LEU:HD22	1.98	0.46
1:A:316:LEU:HD23	1:A:447:ILE:HD13	1.97	0.46
1:D:535:MET:HB2	1:D:540:TYR:O	2.17	0.45
1:A:514:LYS:O	1:A:515:ASP:C	2.55	0.45
1:C:332:THR:O	1:C:433:ILE:HA	2.17	0.45
1:C:531:PHE:O	1:C:544:LYS:NZ	2.48	0.44
1:A:541:LYS:O	1:B:400:SER:HB2	2.19	0.43
1:B:543:MET:HE1	1:B:551:LEU:HD12	2.01	0.42
1:C:325:THR:HB	1:C:451:VAL:HG11	2.02	0.41
1:C:491:ILE:HG21	1:C:529:GLN:HG2	2.02	0.41
1:A:379:SER:HB3	1:A:446:ALA:HB3	2.03	0.40
1:B:457:ASP:HA	1:B:518:LEU:HD21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	298/330 (90%)	280 (94%)	18 (6%)	0	100	100
1	B	285/330 (86%)	276 (97%)	9 (3%)	0	100	100
1	C	295/330 (89%)	282 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	298/330 (90%)	281 (94%)	17 (6%)	0	100	100
All	All	1176/1320 (89%)	1119 (95%)	57 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	277/305 (91%)	277 (100%)	0	100	100
1	B	267/305 (88%)	267 (100%)	0	100	100
1	C	274/305 (90%)	271 (99%)	3 (1%)	80	92
1	D	277/305 (91%)	276 (100%)	1 (0%)	93	98
All	All	1095/1220 (90%)	1091 (100%)	4 (0%)	93	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	278	HIS
1	C	400	SER
1	C	546	TYR
1	D	423	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	547	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	302/330 (91%)	-0.24	1 (0%) 94 94	33, 55, 81, 109	0
1	B	290/330 (87%)	-0.28	4 (1%) 78 77	35, 53, 83, 112	0
1	C	299/330 (90%)	-0.10	3 (1%) 84 83	33, 62, 100, 112	0
1	D	302/330 (91%)	-0.11	5 (1%) 73 72	33, 57, 94, 116	0
All	All	1193/1320 (90%)	-0.18	13 (1%) 82 82	33, 56, 94, 116	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	354	GLY	5.0
1	D	293	LEU	3.4
1	C	474	GLU	2.7
1	D	266	LYS	2.4
1	B	397	LYS	2.3
1	B	395	LEU	2.3
1	B	503	TYR	2.2
1	A	303	ASN	2.2
1	D	503	TYR	2.1
1	B	361	ASN	2.1
1	C	517	LYS	2.0
1	D	510	ILE	2.0
1	C	358	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.